

Singularities in ground state fidelity and quantum phase transitions for the Kitaev model

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The ground state fidelity per lattice site is shown to be able to detect quantum phase transitions for the Kitaev model on the honeycomb lattice, a prototypical example of quantum lattice systems with topological order. It is found that, in the thermodynamic limit, the ground state fidelity per lattice site is non-analytic at the phase boundaries: the second-order derivative of its logarithmic function with respect to a control parameter describing the interaction between neighboring spins is logarithmically divergent. A finite size scaling analysis is performed, which allows us to extract the correlation length critical exponent from the scaling behaviors of the ground state fidelity per lattice site.

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With the advent of its discovery in the fractional quantum Hall effect [1], topological order emerges as a new paradigm in the study of quantum phase transitions (QPTs) [2]. Subsequent investigations show that topological order occurs in various strongly correlated lattice systems undergoing QPTs. A characteristic feature of quantum systems with topological order is their insensitivity to any *local* perturbations [3]. Such an essential difference between topological and symmetry-breaking orders invalidates the usual tools used to describe a symmetry-breaking order, such as long range correlations, broken symmetries, and local order parameters [4].

Recently, much attention has been paid to an exactly solvable spin 1/2 model on a honeycomb lattice introduced by Kitaev [5] for fault-tolerant topological quantum computation [6]. The model describes a set of spins located at the vertices of a two-dimensional honeycomb lattice, subject to a spatially anisotropic interaction between neighboring spins. It has been shown that it carries excitations with both Abelian and non-Abelian braiding statistics, which do not obey ordinary bosonic and fermionic statistics, but are anyons with more intricate statistical behavior [7]. An experimentally feasible realization of the model in a system of cold atoms on an optical lattice has been addressed [8] (see also [9, 10]), with the expectation to perform quantum computation by utilizing braiding of collective excitations implanted in topologically ordered coherent quantum many-body states.

On the other hand, a viable scheme to determine the ground state phase diagram of a quantum lattice system without prior knowledge of order parameters was proposed in Refs. [11, 12, 13, 14]. This was achieved by studying the singularities in the ground state fidelity per lattice site [15]. In fact, the ground state fidelity may be interpreted as the partition function of a classical statistical vertex model with the same lattice geometry by using the tensor network representations of quantum many-body wave functions [12]. Therefore, the fidelity per lattice site is nothing but the partition function per site in the classical statistical vertex lattice model [16]. This justifies why QPTs may be detected as singularities in the fidelity per lattice site as a function of the control parameters (see also Refs. [17, 18] for the connection between the

fidelity and QPTs). Therefore, an intriguing question is to see if the fidelity approach captures the physics underlying QPTs in quantum lattice systems with topological order.

The purpose of this paper is to show that the ground state fidelity per lattice site is able to detect QPTs for the Kitaev model on the honeycomb lattice, a prototypical example of quantum lattice systems with topological order. First, we derive the ground state fidelity per lattice site between different ground states from the exact solution of the Kitaev model on the honeycomb lattice. This is achieved by exploiting the fact that the original spin model on the honeycomb lattice is rephrased as a *p*-wave BCS model with a site-dependent chemical potential for spinless fermions on a square lattice [19] (see also Refs. [20, 21, 22]). The ground state of the latter is a BCS type state, as a consequence of the Jordan-Wigner, Fourier and Bogoliubov transformations. Second, the phase boundaries separating the gapless phase from different gapful phases are reproduced by investigating the singularities in the fidelity per lattice site as a function of the control parameters. It is found that, in the thermodynamic limit, the ground state fidelity per site is non-analytic at the phase boundaries. That is, the second-order derivative of its logarithmic function with respect to a given control parameter is logarithmically divergent as the phase boundaries are crossed. Third, we perform a finite size scaling analysis for the Kitaev model, aiming at extracting the correlation length critical exponent from the scaling behaviors of the ground state fidelity per site. Our exact results offer a benchmark to investigate QPTs for two-dimensional quantum lattice systems with topological order numerically in the context of tensor network representations [23, 24, 25, 26].

The Kitaev model on a honeycomb lattice. Consider a spin 1/2 model on a honeycomb lattice with the Hamiltonian [5]

$$H = -J_x \sum_{x\text{-bonds}} \sigma_i^x \sigma_j^x - J_y \sum_{y\text{-bonds}} \sigma_i^y \sigma_j^y - J_z \sum_{z\text{-bonds}} \sigma_i^z \sigma_j^z, \quad (1)$$

where J_α are interaction (control) parameters and σ_j^α are the Pauli matrices at the site j , with $\alpha = x, y$ and z . The Hamil-

tonian (1) may be fermionized by performing the Jordan-Wigner transformation [19, 20, 21, 22] from the Pauli spin matrices σ_j^α to the spinless fermion operators c_j^\dagger and c_j . This one-dimensional fermionization is realized by deforming the hexagonal lattice into a brick-wall lattice which is topologically equivalent to the original lattice. If we introduce the Majorana fermions: $A = (c - c^\dagger)/i$ and $A = c + c^\dagger$, then the Hamiltonian (1) becomes

$$H = -iJ_x \sum_{x\text{-bonds}} A_w A_b + iJ_y \sum_{y\text{-bonds}} A_b A_w - iJ_z \sum_{z\text{-bonds}} \alpha_r A_b A_w, \quad (2)$$

where the subscripts w and b denote two sublattices in the brick-wall lattice, and $\alpha_r \equiv B_b B_w$ along the z -bond is conserved [20], with r being the coordinate of the midpoint of the bond connecting the b -type and w -type sites. This in turn is equivalent to a model of spinless fermions on a square lattice with a site-dependent chemical potential:

$$H = J_x \sum_r (d_r^\dagger + d_r)(d_{r+\hat{e}_x}^\dagger - d_{r+\hat{e}_x}) + J_y \sum_r (d_r^\dagger + d_r)(d_{r+\hat{e}_y}^\dagger - d_{r+\hat{e}_y}) + J_z \sum_r \alpha_r (2d_r^\dagger d_r - 1). \quad (3)$$

Here the unit vector \hat{e}_x and \hat{e}_y connects two z bonds and crosses a x - and y -bond, respectively. For large enough systems, the ground state configurations are bulk vortex-free configurations [5, 21], which implies $\alpha_r = 1$ for all r . Therefore, the ground state may be obtained by performing a fourier transformation. Up to an unimportant additive constant, the Hamiltonian (3) in the vortex-free configuration now reads,

$$H_g = \sum_k \left(\epsilon_k d_k^\dagger d_k + i \frac{\Delta_k}{2} (d_k^\dagger d_{-k}^\dagger + \text{H.C.}) \right), \quad (4)$$

with $\epsilon_k = 2J_z - 2J_x \cos k_x - 2J_y \cos k_y$, and $\Delta_k = 2J_x \sin q_x + 2J_y \sin k_y$. The Hamiltonian (4) is a p -wave type BCS pairing model and can be diagonalized by means of the Bogoliubov transformation. It yields that the BCS type ground state is $|g\rangle = \prod_k (u_k + v_k d_k^\dagger d_{-k}^\dagger) |0\rangle$, where $|u_k|^2 = 1/2(1 + \epsilon_k/E_k)$ and $|v_k|^2 = 1/2(1 - \epsilon_k/E_k)$, with the quasiparticle excitation energy $E_k = \sqrt{\epsilon_k^2 + \Delta_k^2}$ [19].

The ground state fidelity per lattice site. Consider two ground states $|g\rangle$ and $|g'\rangle$ corresponding to different values of the control parameters $\vec{J} \equiv (J_x, J_y, J_z)$ and $\vec{J}' \equiv (J'_x, J'_y, J'_z)$, respectively. The fidelity $F(\vec{J}; \vec{J}') \equiv \langle g' | g \rangle$ asymptotically scales as $F(\vec{J}; \vec{J}') \sim d(\vec{J}; \vec{J}')^N$, with N the total number of sites in the lattice. Here $d(\vec{J}; \vec{J}')$ is the ground state fidelity per lattice site, introduced in Refs. [11, 12]. Although $F(\vec{J}; \vec{J}')$ becomes trivially zero for continuous QPTs, the fidelity per lattice site is well defined in the thermodynamic limit:

$$d(\vec{J}; \vec{J}') = \lim_{N \rightarrow \infty} F^{\frac{1}{N}}(\vec{J}; \vec{J}'). \quad (5)$$

It satisfies the properties inherited from the fidelity $F(\vec{J}; \vec{J}')$: (i) normalization $d(\vec{J}; \vec{J}) = 1$; (ii) symmetry $d(\vec{J}; \vec{J}') = d(\vec{J}'; \vec{J})$; and (iii) range $0 \leq d(\vec{J}; \vec{J}') \leq 1$.

For the Kitaev model on the honeycomb lattice, the logarithmic function of the fidelity per site, $\ln d_h(\vec{J}; \vec{J}')$, is half of the logarithmic function of the fidelity per site, $\ln d_{sq}(\vec{J}; \vec{J}')$, for the model of spinless fermions on a square lattice. This results from the fact that the number of sites in the honeycomb lattice doubles that of sites in the square lattice. The BCS type ground state $|g\rangle$ yields the ground state fidelity per lattice site for the spinless fermion model on the square lattice:

$$\ln d_{sq}(\vec{J}; \vec{J}') = \frac{1}{(2\pi)^2} \int_0^\pi dk_x \int_0^\pi dk_y \ln(u_k^* u'_k + v_k^* v'_k), \quad (6)$$

where u_k and v_k depend on \vec{J} , whereas u'_k and v'_k depend on \vec{J}' . Here we emphasize that although the information about the topological nature of the Kitaev model is lost in the spinless fermion representation, the unitary equivalence between the two representations preserves the fidelity. Since the extra prefactor does not affect the singularities in $\ln d_h(\vec{J}; \vec{J}')$ and $\ln d_{sq}(\vec{J}; \vec{J}')$, hereafter we focus on $\ln d_{sq}(\vec{J}; \vec{J}')$ to carry out the scaling analysis below, and omit the subscripts for brevity.

For a finite-size system, the Hamiltonian (4), resulted from the Jordan-Wigner, Fourier and Bogoliubov transformations, depends on boundary conditions imposed on the original spin model (1). In contrast to open boundary conditions, there is an extra boundary term if one adopts the periodic boundary conditions. However, such a boundary term does not contribute to the fidelity per site, although it carries the topological dependence of the ground state degeneracy [19]. From now on, we are only concerned with the fermion model on a square lattice with the periodic boundary conditions (i.e., a torus) to analyze the ground state fidelity per lattice site for finite-size systems [27], from which it is sufficient to extract the bulk behaviors of the model. As such, for a system on a torus with an even linear size L , the logarithmic function of the ground state fidelity per lattice site, $\ln d(\vec{J}; \vec{J}')$, takes the form:

$$\ln d(\vec{J}; \vec{J}') = \frac{1}{L^2} \sum_{k_x, k_y} \ln(u_k^* u'_k + v_k^* v'_k). \quad (7)$$

Here k_x and k_y take values from the set: $\pi m/L (m = -(L-1)/2, \dots, (L-1)/2)$, and the double summation is over all positive values of both k_x and k_y .

Ground state phase diagram and singularities in the ground state fidelity per lattice site. Now we turn to the ground state phase diagram. This follows from the singularities in $\ln d(\vec{J}; \vec{J}')$. One may show that $\ln d(\vec{J}; \vec{J}')$ in Eq. (6) and the first-order derivative with respect to a control parameter is continuous, but the second-order derivative logarithmically diverges when the phase boundaries determined by $|J_x| = |J_y| + |J_z|$, $|J_y| = |J_z| + |J_x|$ and $|J_z| = |J_x| + |J_y|$ are crossed. This is consistent with the original analysis by Kitaev [5] (see also Refs. [19, 20, 21]). In Fig. 1(a), we plot the logarithm of the fidelity per site, $\ln d(\vec{J}; \vec{J}')$, as a function of

J_x and J'_x for $J_y = J_z = 1/2$ and $J'_y = J'_z = 1/2$. It is seen that a pinch point occurs at $(J_{xc}, J_{xc}) = (1, 1)$. That is, there are singularities along the lines $J_x = 1$ and $J'_x = 1$. Therefore, the drastic change of the ground state many-body wave functions at J_{xc} is reflected as the singularities in $\ln d(\vec{J}; \vec{J}')$. Similarly, the numerical results are plotted in Fig. 1(b) for the logarithm of the fidelity per lattice site, $\ln d(\vec{J}; \vec{J}')$, as a function of J_z and J'_z for fixed $J_x = J'_x = J_y = J'_y = 1/2$, with a pinch point at $(J_{zc}, J_{zc}) = (1, 1)$.

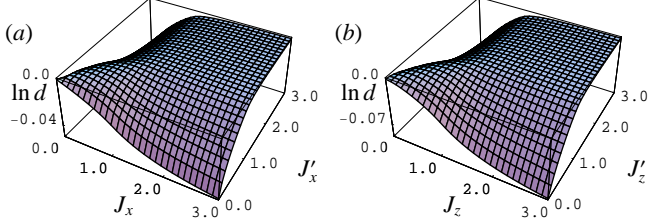


FIG. 1: (color online) (a) The logarithm of the fidelity per lattice site, $\ln d(\vec{J}; \vec{J}')$, is shown as a function of J_x and J'_x for fixed $J_y = J'_y = J_z = J'_z = 1/2$. It exhibits a pinch point at $(J_{xc}, J_{xc}) = (1, 1)$. (b) The logarithm of the fidelity per lattice site, $\ln d(\vec{J}; \vec{J}')$, is shown as a function of J_z and J'_z for fixed $J_x = J'_x = J_y = J'_y = 1/2$. It exhibits a pinch point at $(J_{zc}, J_{zc}) = (1, 1)$. Here a pinch point is defined as an intersection of two singular lines.

More precisely, for any fixed \vec{J}' , $\ln d(\vec{J}; \vec{J}')$ is logarithmically divergent when \vec{J} is varied such that a critical point is crossed. Suppose J_y and J_z are fixed, and only J_x is a control parameter that varies. Then we have

$$\frac{\partial^2 \ln d(\vec{J}; \vec{J}')}{\partial J_x^2} = k_1 \ln |J_x - J_{xc}| + \text{constant}, \quad (8)$$

where k_1 is a non-universal prefactor that depends on J_y, J_z and \vec{J}' , and J_{xc} is the critical value of J_x for fixed J_y and J_z . The numerical results are plotted in Fig. 2(a) for $J_y = J_z = 1/2$ and $J_{xc} = 1$. The least square fit yields $k_1 \approx 0.02360$. Similarly, we have presented numerics in Fig. 2(b) for the second-order derivative of $\ln d(\vec{J}; \vec{J}')$ with respect to J_z , with $J'_z = 0.8$ and $J_x = J'_x = J_y = J'_y = 1/2$. It turns out that it diverges logarithmically in the same way as (8) with J_x replaced by J_z , and $k_1 \approx 0.04726$.

Finite size scaling analysis. For a system of finite size $N \equiv L^2$ (with L the linear size), there is no divergence in the second-order derivative of $\ln d(\vec{J}; \vec{J}')$ with respect to J_x , since QPTs only occur in the thermodynamic limit. Instead, as seen in Fig. 2(a), some pronounced dips occur at the so-called quasi-critical points J_{xm} , with the dips values logarithmically diverging with increasing linear size L ,

$$\left. \frac{\partial^2 \ln d(\vec{J}; \vec{J}')}{\partial J_x^2} \right|_{J_x=J_{xm}} = k_2 \ln L + \text{constant}, \quad (9)$$

where k_2 is a non-universal prefactor k_2 , which takes the value $k_2 \approx -0.02312$ for $J'_x = 0.8$ and $J_y = J'_y = J_z = J'_z = 1/2$

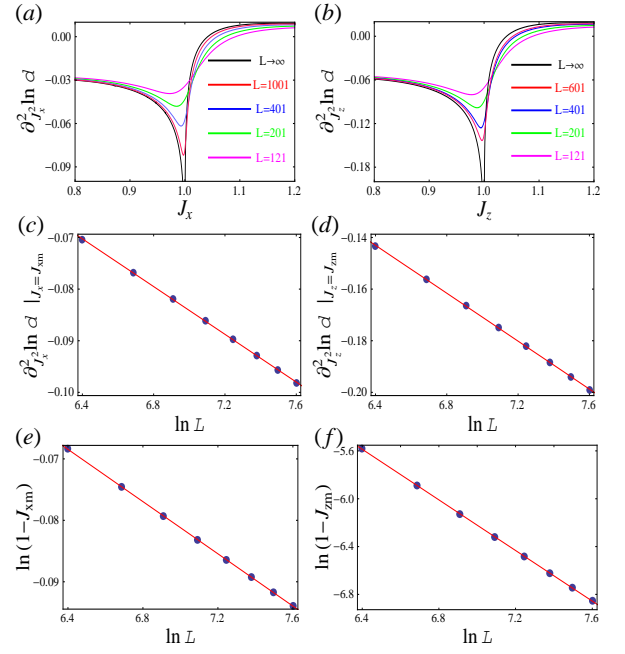


FIG. 2: (color online) (a) The second-order derivative of the logarithm of the fidelity per lattice site, $\ln d(\vec{J}; \vec{J}')$, with respect to J_x diverges at the critical point in the thermodynamic limit. However, it remains analytic for finite-size systems, although more pronounced dips occur with increasing linear system size. Here $J'_x = 0.8$ and $J_y = J'_y = J_z = J'_z = 1/2$. (b) The second-order derivative of the logarithm of the fidelity per lattice site, $\ln d(\vec{J}; \vec{J}')$, with respect to J_z diverges at the critical point in the thermodynamic limit. However, it remains analytic for finite-size systems, although more pronounced dips occur with increasing linear system size. Here $J'_z = 0.8$ and $J_x = J'_x = J_y = J'_y = 1/2$. (c) The dips values scale as $\ln L$ with increasing linear size L for $J'_x = 0.8$ and $J_y = J'_y = J_z = J'_z = 1/2$. (d) The dips values scales as $\ln L$ with the linear size L for $J'_z = 0.8$ and $J_x = J'_x = J_y = J'_y = 1/2$. (e) The positions of the dips approach the critical point $J_{xc} = 1$ with increasing linear size L . Here $d(\vec{J}; \vec{J}')$ is shown as a function of J_x for $J'_x = 0.8$ and $J_y = J'_y = J_z = J'_z = 1/2$. (f) The positions of the dips approach the critical point $J_{zc} = 1$ with increasing linear size L . Here $d(\vec{J}; \vec{J}')$ is shown as a function of J_z for $J'_z = 0.8$ and $J_x = J'_x = J_y = J'_y = 1/2$.

(see Fig. 2(c)). In addition, J_{xm} approaches the critical value as $J_{xm} \sim 1 - 3.96384L^{-1.06245}$, as follows from Fig. 2(e). The scaling ansatz in the system exhibiting logarithmic divergences requires that the absolute value of the ratio k_1/k_2 is the correlation length critical exponent ν . In this case, $|k_1/k_2| \sim 1.02076$, very close to the exact value $\nu = 1$. This is consistent with the fact that the gap Δ for the Bogoliubov quasiparticle scales as $\Delta \sim J_x - J_{xc}$ near the critical point J_{xc} . Similarly, a finite size scaling analysis is performed for $\ln d(\vec{J}; \vec{J}')$ with $J'_z = 0.8$ and $J_x = J'_x = J_y = J'_y = 1/2$. In Fig. 2(c), the least square fit yields $k_2 \approx -0.04640$. The numerics for $\partial^2 \ln d(\vec{J}; \vec{J}') / \partial J_x^2|_{J_x=J_{xm}}$ and J_{xm} are plotted in Figs. 2(d) and (f), respectively.

In order to address the scaling ansatz for a system exhibiting logarithmic divergence [28], we take into account the distance of the minimum of $\partial^2 \ln d(\vec{J}; \vec{J}')$ from the critical point

to investigate $1 - \exp[\partial_{J_x}^2 \ln d(\vec{J}, \vec{J}) - \partial_{J_x}^2 \ln d(\vec{J}, \vec{J})|_{J_x=J_{xm}}]$ as a function of $L(J_x - J_{xm})$ for different linear sizes L 's. The numerical results for the linear size ranging from $L = 401$ up to $L = 1401$ are plotted in Fig. 3(a). All the data for different L 's collapse onto a single curve, indicating that the model is scale invariant, i.e., $\xi/L = \xi'/L'$, and that the correlation length critical exponent $\nu = 1$. The same conclusion can be drawn from Fig. 3(b), where the data collapsing is confirmed for $1 - \exp[\partial_{J_z}^2 \ln d(\vec{J}, \vec{J}) - \partial_{J_z}^2 \ln d(\vec{J}, \vec{J})|_{J_z=J_{zm}}]$.

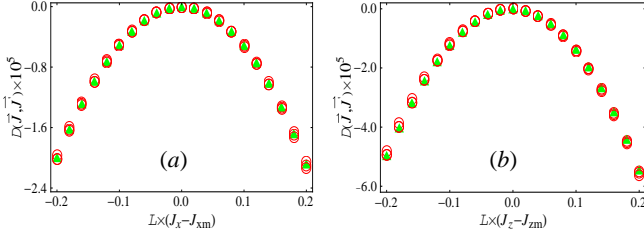


FIG. 3: (color online) (a) A finite size scaling analysis is performed for a quantity defined as $D(\vec{J}, \vec{J}) = 1 - \exp[\partial_{J_x}^2 \ln d(\vec{J}, \vec{J}) - \partial_{J_x}^2 \ln d(\vec{J}, \vec{J})|_{J_x=J_{xm}}]$, with J_y, J_z and \vec{J} fixed. The scaling ansatz for logarithmic divergences implies that $D(\vec{J}, \vec{J})$ is a function of $L(J_x - J_{xm})$ for fixed J_y, J_z and \vec{J} . (b) A finite size scaling analysis is performed for a quantity defined as $D(\vec{J}, \vec{J}) = 1 - \exp[\partial_{J_z}^2 \ln d(\vec{J}, \vec{J}) - \partial_{J_z}^2 \ln d(\vec{J}, \vec{J})|_{J_z=J_{zm}}]$, with J_x, J_y and \vec{J} fixed. The scaling ansatz implies that $D(\vec{J}, \vec{J})$ is a function of $L(J_z - J_{zm})$ for fixed J_x, J_y and \vec{J} . All the data from $L = 401$ up to $L = 1401$ collapse onto a single curve. This shows that the system at a critical point is scale invariant and that the correlation length critical exponent ν is 1.

Summary. We have demonstrated that the ground state fidelity per lattice site is able to detect QPTs in the Kitaev model on the honeycomb lattice. It is found that, in the thermodynamic limit, the ground state fidelity per lattice site is non-analytic at a critical point. More precisely, the second-order derivative of its logarithmic function with respect to a given control parameter is logarithmically divergent as the phase boundaries are crossed. A finite size scaling analysis has also been performed to extract the correlation length critical exponent from the scaling behaviors of the fidelity per site. Our exact results offer a benchmark to numerically investigate QPTs for two-dimensional quantum lattice systems with topological order in the context of tensor network representations, which is currently under investigation.

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